mar research

The

mar345
Software Guide

By Dr. Claudio Klein

The *mar345* Software Guide

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Contents

1. Distribution Media

Media	OS	Suggested directory	Mount CD–Rom with
CD–Rom	IRIX 5.x,6.x DEC Unix 5.0 Linux, 2.0.x	/usr/people/mar345 /usr/users/mar345 /home/mar345	mount –t iso9660 –r /dev/rdsk/dksXdYvol /CDROM mount –t iso9660 –r –o rrip /dev/rzYc /mnt mount –t is09660 –r /dev/cdrom /mnt/cdrom

X denotes the SCSI–controller (e.g.0) and Y the SCSI–id (e.g. 4).
Most executable programs are also available as gzip compressed files via anonymous FTP from ftp.EMBL–Hamburg.de, directory pub/marx/mar345/.... Due to their size (180 MB), scanner calibration files are not available per FTP. Please contact X–ray Research for assistance.

2. Compilation Notes

OS	Compilers used	Motif version used	
IRIX	C–7.1	Motif 1.2.4	X11R6
DEC Unix	C–5.2	Motif 1.2.4	X11R5
Linux	GCC–2.7.2	Motif 2.1.x	X11R6

3. Environment

The following logicals assigments must be set to run certain programs:

Variable	Description	Used by
MARHOME	Master directory of software distribution.	–
MARLOGDIR	Directory where log files will be created.	*mar345, mar345xf, scan345, marHKL*
MARMANDIR	Directory with man pages.	–
MARHELPDIR	Directory with online help files.	*mar345, marView marTools*
MARTABLEDIR	Directory with scanner specific tables.	*mar345, mar345xf, scan345*
MAR_SCANNER_NO	Scanner serial number.	*mar345, mar345xf, scan345*

4. Directory Structure

The **mar345** software distribution directory ($MARHOME) contains the following subdirectories:

Subdirectory	Contents
bin/sgi **bin/osf** **bin/linux**	Binary executables for corresponding platforms.
man/1 **man/cat1** **man/man1** **man/ps** **man/doc** **man/help**	Unformatted man pages for selected programs. Formatted man pages (SGI). Compressed unformatted man pages (Linux & DEC Unix). Postscript files of formatted man pages, ready for printing. ASCII text of formatted man pages, ready for online read (more). Online help files for GUI's (*mar345,marView, marTools*).
log **log/log** **log/lp** **log/spy** **log/sets**	Log–files for programs *mar345* and *scan345*. Up to 99 versions of mar.log files. Up to 99 versions of mar.lp files (statistical output). Up to 99 versions of mar.spy files (native controller messages). Data collection strategy template files for *mar345*.
src **tables**	Source code of selected programs. Scanner specificic calibration and configuration files.
Optional: **marflm** **marhkl** **marxds**	Latest *marFLM* distribution. Latest *marHKL* distribution. Latest *marXDS* distribution.

5. Description of Programs

Name	man page	Priority	Description
Graphical User Interfaces:			
mar345	mar345	A	GUI for data collection and display.
marstart	–	A	Works together with program *mar345* and must be available.
marView	marView	A	GUI for data display.
marTools	marTools	A	GUI for image file manipulation: format conversion, etc.
tkmarcvt	tkmarcvt	A	GUI for image format conversion. Relies on Tcl/Tk package (not installed in a standard SGI installation).
marHKL	–	B	GUI for HKL processing package (DENZO, xdisp).
marFLM	–	B	GUI for MOSFLM processing package.
marXDS	–	B	GUI for XDS processing package (XDS, xscale).
Hardware related programs:			
mar345xf	mar345xf	C	Standalone transformation program for spiral images.
marsim	marsim	D	Scanner simulator. Works together with programs *mar345* or *scan345*. This is for performance tests and/or debugging.
scan345	scan345	D	Non–GUI data collection program: no display, no goniometer functions, just scans and spiral to Cartesian conversion.
modnb	–	D	Modifies header of calibration files.
swapnb	–	D	Swaps bytes in calibration file. Useful when replacing the data collection computer by one with a different byte–order.
Format conversion programs:			
marcvt	marcvt	A	Conversion of *mar345* formats into other formats. Also used by tkmarcvt (see above).
spiral(un)pack	spiralpack	C	(De–)Compression of spiral images as produced by *mar345*.
Others:			
catmar	catmar	B	Dumps image header (*mar345* and *mar300* formats, also for calibration files).
marstats	–	C	Dumps average intensity and sigmas of images.
Data processing related programs for use within *marHKL, marFLM* and *marXDS*:			
marPeaks	marPeaks	B	Spot search program.
marIndex	marIndex	B	Autoindexing program (based on marPeaks).
marPredict	marPredict	B	Pattern prediction program (based on marIndex).
marStrategy	marStrategy	B	Program to calculate an optimal data collection strategy.

Priority codes:

A	Essential
B	Helpful, installation recommended
C	Not essential, may be removed
D	Needed only in special situations.

6. Documentation

The documentation can be found in directory $MARHOME/man. Several formats are available:

Directory	Description
man/1	Unformatted man pages for selected programs.
man/cat1	Formatted man pages (SGI).
man/man1	Compressed unformatted man pages (Linux & DEC Unix).
man/ps	Postscript files of formatted man pages, ready for printing.
man/doc	ASCII text of formatted man pages, ready for online read (*more*).
man/help	Online help files for GUI's (*mar345,marView, marTools*).

The following man pages are available:

Name	Description
Programs:	
mar345	Documentation for program *mar345*.
marView	Documentation for program *marView*.
marTools	Documentation for program *marTools*.
tkmarcvt	Documentation for program *tkmarcvt*.
mar345xf	Documentation for program *mar345xf*.
scan345	Documentation for program *scan345*.
marsim	Documentation for program *marsim*.
marcvt	Documentation for program *marcvt*.
spiralpack	Documentation for program *spiralpack*.
catmar	Documentation for program *catmar*.
marPeaks	Documentation for program *marPeaks*.
marIndex	Documentation for program *marIndex*.
marPredict	Documentation for program *marPredict*.
marStrategy	Documentation for program *marStrategy*.
Others:	
mar345_formats	Documentation for *mar345* image formats.
mar300_formats	Documentation for *mar300* image formats.
mar345_config_file	Documentation for the config file entries for program *mar345*.

To view the man pages using man, the directory $MARHOME/man must be in the man page search path. Consult the "man" man page for further details, since this varies from computer to computer.

The GUI's provide "Help"–buttons for additional online information.

When run with the "–h" command line option, usage information is provided for most of the mar programs, e.g. type:

        marcvt –h

7. Installation on SGI IRIX

7.1 Installing the Software (IRIX 6.5)

7.1.1 Login as user "root" and create a new user account called *mar345.*
Do the following:
   a) From the toolchest (usually in the upper left corner of the screen) choose "**System Manager**" from the "**System**" menu.
   b) In the main window of the "**System Manager**", choose: "**Security and Access Control...**"
   c) Select "**Add a User Account**" and go through steps 1 to 10.
      Choose "**mar345**" as "**Login name**" (suggested).
      Choose "**Password**", "**User–ID**" and "**Primary Group**" as desired.
      Choose "**/usr/people/mar345**" as "**Home Directory**" (suggested).
      Choose "**tcsh**" as "**Shell Program**" (strongly recommended).
      As a last step, press "**OK**" to accept the settings.

7.1.2 Login as user: **mar345**

7.1.3 Installing the software from CD–ROM:

Insert the CD–ROM in the CD–ROM reader. After a couple of seconds, the automounter should mount the CD automatically as /CDROM. If not, the super–user should try:

mount –t iso9660 –r /dev/rdsk/dks0d4vol /CDROM

where 4 is the SCSI–unit number of the CD–ROM on the system, which may vary. If you are not certain, which SCSI–unit your CD–ROM drive uses, try comand:
         hinv
to get a "hardware inventory" of your system which will say something like:
         CDROM: unit 4 on SCSI controller 0:

When successful, the contents of the CD–ROM should be copied into the login directory of the account mar345.To do so, as user "mar345" type:

/CDROM/mar_install

The installation script chooses reasonable defaults that may be accepted or modified.
It is important that the contents of the CD–Rom are really copied to the login directory of the new user since the distribution contains customized startup files (.cshrc, etc.) which should reside in the login directory.

7.1.2 Setting Up the Ethernet Connection

The scanner control program *mar345* communicates with the scanner through a Ethernet interface. To use *mar345*, the network must be configured to meet the requirements of the mar controller.The mar scanner will respond only to requests made to IP–address 192.0.2.1. The mar scanner also requires the host computer Ethernet interface to be set to address 192.0.2.2. These addresses belong to a pool of addresses that are not assigned to official networks so there should not be any conflict with the outside world.
Do the following:

7.1.2.1 Edit file /etc/hosts, e.g. type:
>   **jot   /etc/hosts**
and add the following line to the end of the file:
>   **192.0.2.1   mar345**
>   **192.0.2.2   gate–$HOSTNAME**
where $HOSTNAME is the original name of your computer, e.g. if the computer is called "mars", then write:
>   **192.0.2.2   gate–mars**

7.1.2.2 If the second network interface is not yet configured, edit file /etc/config/netif.options:
>   **jot   /etc/config/netif.options**
and modify lines:
>   **: if2name=**
>   **: if2addr=gate–$HOSTNAME**
to:
>   **if2name=ec1**
>   **if2addr=gate–$HOSTNAME**

7.1.2.3 Reboot.

7.1.2.4 Check settings

The second network interface (ec1) should now be configured and you should be able to access other hosts (e.g mar345) on network 192.0.2. To check, type:
>   **/usr/etc/ifconfig   ec1**
This command should come back with something like:
ec2: flags=c63<UP,BROADCAST,NOTRAILERS,RUNNING,FILTMULTI,MULTICAST>
>   **inet 192.0.2.2 netmask 0xffffff00 broadcast 192.0.2.255**

The correct routing table can be checked using command:
>   **netstat –rn**
It should say something like:

Destination	Gateway	Netmask	Flags	Refs	Use	Interface
default	192.168.0.1		UGS	1	0	ec0
127.0.0.1	127.0.0.1		UH	5	592	lo0
192.0.2	link#1	0xffffff00	UC	0	0	ec1
192.168	link#2	0xffffff00	UC	0	0	ec0
196.168.0.3	127.0.0.1		UGHS	2	2	lo0
224	link#2	0xffffff00	UCS	0	0	ec0
255.255.255.255	192.168.0.255		UGHS	0	0	ec0

To manually configure ec1, type:
>   **/usr/etc/ifconfig   ec1   inet 192.0.2.2**
>   **route add net 192.0.2.0 gate–$HOSTNAME 0**

Note: You may also use the graphical system configuraton tools ("**System**" –> "**System Manager**" –> "**Network and Connectivity**" –> "**Network Interface Manager**" –> "**Ethernet ec1**") to configure the second Ethernet card. In practice, the GUI's have failed so many times, that it seems much easier to do the steps 7.1.2.1 and 7.1.2.2 manually.

8. Installation on DEC Unix

8.1 Installing the Software (DEC Unix 4.0)

8.1.1 Create a new user account called *mar345.*
   Type:
   a) **su**   = become superuser
   b) **/usr/bin/X11/dxaccounts**   = call the "Account Manager" graphical interface
   c) In the main window of the "**Account Manager**", choose: "**Add...**"
   d) In the window "**Create/Modify Local User**" fill in at least the "**User name**" and "**Shell**" press "**OK**".
      As default shell, the "/bin/tcsh" is recommended. However, the "tcsh" is not installed by default on
      DEC Unix 4.0. If "tcsh" is unavailable (look also in /usr/bin and /usr/local/bin) choose: "**/bin/csh**".
      As "**Home Directory**" use of **/usr/users/mar345** is suggested. At this time you may create a
      password for this user account but you don't have to. All other fields do not need to be modified.
      Press "**OK**" to accept the settings.
   f) Press "**Close**" to leave the "**Account Manager**".
   g) Log out.

8.1.2 Login as user: **mar345**

8.1.3 Installing the software from CD-ROM:

   Insert the CD-ROM in the CD-ROM reader. Since normally there is no automounter, the mounting
   probably needs to be done as super-user. Type:

   mount -t cdfs -o rrip -r /dev/rz0c /mnt

   When successful, the contents of the CD-ROM should be copied into the login directory of the
   account mar345.To do so, as user "mar345" type:

   /mnt/mar_install

   The installation script chooses reasonable defaults that may be accepted or modified.
   It is important that the contents of the CD-Rom are really copied to the login directory of the new
   user since the distribution contains customized startup files (.cshrc, etc.) which should reside in the
   login directory.

8.2 Setting Up the Ethernet Connection

The scanner control program *mar345* communicates with the scanner through a Ethernet interface. To use *mar345*, the network must be configured to meet the requirements of the mar controller.The mar scanner will respond only to requests made to IP–address 192.0.2.1. The mar scanner also requires the host computer Ethernet interface to be set to address 192.0.2.2. These addresses belong to a pool of addresses that are not assigned to official networks so there should not be any conflict with the outside world.
Do the following:

8.2.1 Configure the second Ethernet card (tu1)
Type:

1.) **su**	= become superuser
2.) **/usr/sbin/netconfig**	= call the "Network Configuration" GUI
3.) Choose "**Ethernet Interface – tu1**"	
4.) Select: "**tu1 – Interface Configuration:**"	**Enable**
5.) Enter "**Host name:**"	**marcontrol**
6.) Enter "**IP address:**":	**192.0.2.2**
7.) Enter: "**Network Mask**":	**255.255.255.0**
8.) Press:	**Commit**

8.2.2 Edit file /etc/hosts, e.g. type:
        vi   /etc/hosts
and add the following line to the end of the file:
        192.0.2.1   mar345
If you can't find an entry for name marcontrol, also add:
        192.0.2.2   marcontrol

8.2.3 Close the "**Network Configuration**" GUI.

The second network interface (tu1) should be configured now and you should be able to access other hosts (e.g mar345) on network 192.0.2. To check, type:
        ifconfig tu1
This command should come back with something like:

tu1:   **flags=c63<UP,BROADCAST,NOTRAILERS,RUNNING,MULTICAST,SIMPLEX>**
                inet 192.0.2.2 netmask ffffff00 broadcast 192.0.2.255 ipmtu 1500

The correct routing table can be checked using command:
        netstat –r
It should say something like:
Routing tables

Destination	**Gateway**	**Flags**	**Refs**	**Use**	**Interface**
Netmasks:					
Inet	**255.255.255.0**				
localhost	**localhost**	**UH**	**5**	**592**	**lo0**
192.0.2	**marcontrol**	**U**	**1**	**0**	**tu1**
193.141.161	**cal**	**U**	**47**	**779**	**tu0**

8.2.4 Connect the scanner to the second Ethernet card and power it up.

9. Installation on Linux (RedHat Distribution)

9.1 Installing the Software

9.1.1 Create a new user account called *mar345.*
Type:
a) **su**   = become superuser
b) **adduser mar345**   = adds user account "mar345" using defaults.
c) Edit **/etc/passwd** and change the default shell of user "**mar345**" to "**/bin/tcsh**".
   Possibly, the password of account "**mar345**" has to be set.

9.1.2 Login as user: **mar345**

9.1.3 Installing the software from CD-ROM:

Insert the CD-ROM in the CD-ROM reader. If there is an automounter, the CD-Rom is going to be
mounted automatically (on RedHat usually as /mnt/cdrom). Otherwise, on many Linux system, users
are allowed to mount CD-Roms by just typing:

            mount   **/mnt/cdrom**   **(RedHat)**
or
            mount   **/cdrom**   **(SuSE)**

If this doesn't work, the super-user has to do something like:

            mount –t iso9660   –r /dev/cdrom /mnt/cdrom

When successful, the contents of the CD-ROM should be copied into the login directory of the
account mar345.To do so, as user "mar345" type:

            /mnt/cdrom/mar_install

The installation script chooses reasonable defaults that may be accepted or modified.
It is important that the contents of the CD-Rom are really copied to the login directory of the new
user since the distribution contains customized startup files (.cshrc, etc.) which should reside in the
login directory.

9.2 Setting Up the Ethernet Connection

The scanner control program *mar345* communicates with the scanner through a Ethernet interface. To use
mar345, the network must be configured to meet the requirements of the mar controller.The mar scanner will
respond only to requests made to IP–address 192.0.2.1. The mar scanner also requires the host computer
Ethernet interface to be set to address 192.0.2.2. These addresses belong to a pool of addresses that are not
assigned to official networks so there should not be any conflict with the outside world.
Do the following:

9.2.1 Configure the second Ethernet card (eth1)
    Type:
      1.) **su**   = become superuser
      2.) **/usr/bin/netcfg**   = call the "Network Configuration" GUI
      3.) Choose section "**Interfaces**"
      4.) Choose button "**Add**"
      5.) Choose "**Interface Type:**"   **Ethernet**
      6.) In window "**Edit Ethernet/Bus Interfaces**"
          Enter: "**IP**":   **192.0.2.2**
          Enter: "**Netmask**":   **255.255.255.0**
          Select: "**Activate interface at boot time**"
      8.) Press: **Done**
      9.) Confirm: **Save configuration**
      10.) In main window, select interface "eth1" and click button "**Activate**"
      11.) Click button "**Save**" and "**Quit**".

For the kernel to actually initialize 2 Ethernet cards, please consult the documentation of the Linux boot load "**lilo**", i.e. read the lilo man page or the lilo documentation in /usr/doc/lilo*.

Note: On SuSE systems, the integration of the second Ethernet card is done via the SuSE system administration tool (yast or yast2). Program netcfg is not available.

9.2.2 Edit file /etc/hosts, e.g. type:
               vi   /etc/hosts
and add the following line to the end of the file:
               192.0.2.1   mar345
If you can't find an entry for name marcontrol, also add:
               192.0.2.2   marcontrol

The second network interface (eth1) should be configured now and you should be able to access other hosts (e.g mar345) on network 192.0.2. To check, type:
               ifconfig   eth1
This command should come back with something like:

eth1   **Link encap:10Mbps Ethernet HWaddr 00:80:C6:FF:EF:08**
                      inet addr:192.0.2.2 Bcast:192.0.2.255 Mask:255.255.255.0
                      UP BROADCAST RUNNING MULTICAST MTU:1500 Metric:1
                      RX packets:0 errors:0 dropped:0 overruns:0
                      TX packets:0 errors:0 dropped:0 overruns:0
                      Interrupt:12 Base address:0x320

The correct routing table can be checked using command:
               netstat –r
It should say something like:

Kernel IP routing table

Destination	Gateway	Genmask	Flags	MSS	Window	irtt	Iface
193.141.161.0	*	255.255.255.0	U	1500	0	0	eth0
192.0.2.0	*	255.255.255.0	U	1500	0	0	eth1
127.0.0.0	*	255.0.0.0	U	3584	0		

9.2.3 Connect the scanner to the second Ethernet card and power it up.

10. Running mar345

10.1 Turn the scanner on. Wait until you hear the plate locking sound (click!).

10.2 Login as user mar345.

10.3 Try to talk to the scanner, i.e. type:

ping mar345 or **/usr/etc/ping mar345 (SGI)**

If the scanner is accessible, ping comes back with:

PING mar345 (192.0.2.1): 56 data bytes
64 bytes from 192.0.2.1: icmp_seq=0 ttl=255 time=1 ms

...

If ping comes back with:

ping: mar345: Unknown host

then, mar345 has not been inserted into file /etc/hosts (see 2.1).
If ping hangs with:

PING 192.0.2.1 (192.0.2.1): 56 data bytes

then the reason might be
a) the interface has not been configured correctly.
b) the scanner is not turned or not yet ready to listen.
c) there is a problem with the Ethernet cable.
d) there is a problem with the T–connectors.
e) there is a problem with the scanner itself.

10.4 In a terminal window, type "**go**" to start the mar software (**mar345**).